3rd ANNUAL COORDINATION MEETING OF THE DOE COMPUTATIONAL MATERIALS AND CHEMICAL SCIENCE NETWORK (CMCSN) ON “PREDICTIVE MODELING OF THE GROWTH AND PROPERTIES OF ENERGY-RELEVANT THIN FILM AND NANOSTRUCTURES”

January 20 – 22, 2011

Room 3.204, Natural Science and Engineering Research Laboratory (RL), University of Texas at Dallas, TX

CMCSN Coordinators: Kai-Ming Ho (Iowa State U & Ames Lab) Zhenyu Zhang (U Tennessee)

Scientific Committee: Chair: Yves Chabal (UT Dallas)
KJ Cho (UT Dallas); Bob Helms (UT Dallas); David Langreth (Rutgers U)
Kai-Ming Ho (ISU); Cai-Zhuang Wang (Ames Lab); Zhenyu Zhang (U Tennessee)

Program

Thursday January 20

2:00-2:30 pm Opening remarks & welcome Yves Chabal and Bob Helms

Session I Nonequilibrium Growth Chair: K.J. Cho (UT Dallas)
2:30-3:00 pm Ted Einstein (U Maryland) - Ordering of giant molecular honeycomb networks: closed-shell quantum dots or metallic surface states?
3:00-3:30 pm Jim Evans (Ames Lab/ISU) - Far-from-equilibrium growth of epitaxial metal nanostructures in multicomponent systems: Predictive atomistic modeling
3:30-4:00 pm Feng Liu (U Utah) - Non-equilibrium compositions of alloy quantum dots and its correlation with growth mode

4:00-4:20 pm Coffee Break

Session II Graphene Chair: Michael Tringides (ISU)
4:20-4:50 pm Phil First (Georgia Tech) - Quantized states of electrons in epitaxial graphene
4:50-5:20 pm Myron Hupalo (Ames Lab) - Metals on graphene: preparation and growth
5:20-5:50 pm Cai-Zhuang Wang (Ames Lab) - Adsorption of metal atoms on graphene by first-principles calculations

6:00 pm Reception and pizza (Remarks by Mark Spong, Dean of the Erik Jonsson School of Engineering)

Friday January 21

Session III Water on Surface Chair: Yves Chabal (UT Dallas)
8:30-9:00 am Adri van Duin (Penn State) - Development and application of ReaxFF reactive force fields to model surface chemistry
9:00-9:30 am Peter Feibelman (Sandia) - Structure of water monolayers on close-packed precious metals
9:30-10:00 am Annabella Selloni (Princeton U) - Structure, defects and water adsorption on TiO2 surfaces

10:00-10:30 am Coffee Break
<table>
<thead>
<tr>
<th>Session IV</th>
<th>Metal on Semiconductor</th>
<th>Chair: Zhenyu Zhang (U Tennessee)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10:30-11:00 am</td>
<td><em>Pat Thiel</em> (Ames Lab/SU)</td>
<td>Ag on Si(111): An Old System with New Surprises</td>
</tr>
<tr>
<td>11:00-11:30 am</td>
<td><em>Jim Chelikowsky</em> (UT Austin)</td>
<td>The evolution of Schottky barriers in metal-semiconductor nanofilms</td>
</tr>
<tr>
<td>11:30am-12:00pm</td>
<td><em>Kai-Ming Ho</em> (ISU/Ames Lab)</td>
<td>Coverage Dependent Collective Diffusivity of Dense Pb Wetting Layer on Si(111)</td>
</tr>
<tr>
<td>12:00-1:30 pm</td>
<td>Lunch Break</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Session V</th>
<th>Catalysis and Multiscale Modeling</th>
<th>Chair: Bob Helms (UT Dallas)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:30-2:00 pm</td>
<td><em>Yves Chabal</em> (UT Dallas)</td>
<td>Molecular Hydrogen dissociation on Ti-doped Aluminum surfaces</td>
</tr>
<tr>
<td>2:00-2:30 pm</td>
<td><em>Sok Pantelides</em> (Vanderbilt U)</td>
<td>Energy issues: Nanocatalysis and battery materials</td>
</tr>
<tr>
<td>2:30-3:00 pm</td>
<td><em>Alain Esteve</em> (Toulouse, France)</td>
<td>Multiscale modelling issues in nanoenergetic materials engineering</td>
</tr>
<tr>
<td>3:00-3:30 pm</td>
<td>Coffee Break</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Session VI</th>
<th>Plasmonics &amp; Solar Cells</th>
<th>Chair: Kai-Ming Ho (ISU/Ames Lab)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3:30-4:00 pm</td>
<td><em>Peter Nordlander</em> (Rice U)</td>
<td>Plasmonic enhancements of light-matter interactions</td>
</tr>
<tr>
<td>4:00-4:30 pm</td>
<td><em>Ken Shih</em> (UT Austin)</td>
<td>Ultra-low Damping of Surface Plasmon Polaritons in Atomically Smooth Epitaxial Ag Films</td>
</tr>
<tr>
<td>4:30-5:00 pm</td>
<td><em>Zhenyu Zhang</em> (U Tennessee)</td>
<td>Quantum tuning of plasmonics for enhanced solar energy conversion</td>
</tr>
<tr>
<td>5:00-5:30 pm</td>
<td><em>Efthimios Kaxiras</em> (Harvard U)</td>
<td>First-principles simulations of hybrid organic-inorganic devices for photovoltaic applications: predictions of efficiency and stability</td>
</tr>
<tr>
<td>6:30 pm</td>
<td>Dinner Reception (Hyatt Hotel)</td>
<td></td>
</tr>
</tbody>
</table>

**Saturday January 22**

<table>
<thead>
<tr>
<th>Session VII</th>
<th>Oxides</th>
<th>Chair: David Langreth (Rutgers U)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30-9:00 am</td>
<td><em>Gyula Eres</em> (ORNL)</td>
<td>Bandgap narrowing of titanium oxide semiconductors by non-compensated anion-cation codoping for enhanced visible-light photoactivity</td>
</tr>
<tr>
<td>9:00-9:30 am</td>
<td><em>Norman Mannella</em> (U Tennessee)</td>
<td>Recent x-ray spectroscopy results in non-compensated doped TiO₂</td>
</tr>
<tr>
<td>9:30-10:00 am</td>
<td><em>Shengbai Zhang</em> (RPI)</td>
<td>Optimal doping of SiO₂</td>
</tr>
<tr>
<td>10:00-10:30 am</td>
<td><em>Lingzhu Kong</em> (Princeton U)</td>
<td>Rotational-vibrational frequencies and infrared intensity for van der Waals bonded H₂ in nanoporous materials</td>
</tr>
<tr>
<td>10:30-10:45 am</td>
<td>Coffee Break</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Session VIII</th>
<th>Theory &amp; Modeling</th>
<th>Chair: Jim Chelikowsky (UT Austin)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10:45-11:15 am</td>
<td><em>Suhuai Wei</em> (NREL)</td>
<td>Theoretical study of pseudo-quaternary Cu₉ZnSn(S,Se)₄ alloy for thinfilm solar cell applications</td>
</tr>
<tr>
<td>11:15-11:45 am</td>
<td><em>Qiming Zhang</em> (UT Arlington)</td>
<td>Amphoteric conductivity of Cu₉O: first-principles studies</td>
</tr>
<tr>
<td>11:45am-12:15pm</td>
<td><em>K.J. Cho</em> (UT Dallas)</td>
<td>Multiscale design of metal alloy catalysts for clean energy applications</td>
</tr>
<tr>
<td>12:15-12:30 pm</td>
<td>Closing Remarks</td>
<td>Kai-Ming Ho &amp; Shengbai Zhang</td>
</tr>
<tr>
<td>12:30-3:00 pm</td>
<td>Lunch and CMCSN meeting</td>
<td></td>
</tr>
</tbody>
</table>